

# A large class of bound-state solutions of the Schrödinger equation via Laplace transform of the confluent hypergeometric equation<sup>a</sup>

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## Abstract

It is shown that analytically soluble bound states of the Schrödinger equation for a large class of systems relevant to atomic and molecular physics can be obtained by means of the Laplace transform of the confluent hypergeometric equation. It is also shown that all closed-form eigenfunctions are expressed in terms of generalized Laguerre polynomials. The generalized Morse potential is used as an illustration.

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## I. INTRODUCTION

Some exactly soluble systems with importance in atomic and molecular physics have been approached in the literature on quantum mechanics with a myriad of methods. Among such systems is the Morse potential  $a(e^{-\alpha x} - 2e^{-2\alpha x})$  [1]-[19], the pseudoharmonic potential  $a(x/b - b/x)^2$  [4]-[5], [20]-[31], and the Kratzer-Fues potential  $a(b^2/x^2 - 2b/x)$  and its modified version  $a(b^2/x^2 - b/x)$  [4]-[5], [12], [30]-[34]. More general exactly soluble systems have also been appreciated: the generalized Morse potential  $Ae^{-\alpha x} + Be^{-2\alpha x}$  [31], [35]-[39], the singular harmonic oscillator  $Ax^2 + Bx^{-2}$  [3]-[5], [19], [36], [40]-[52], the singular Coulomb potential  $Ax^{-1} + Bx^{-2}$  [2]-[5], [36], [40], [48], [50]-[51], [53]-[57], and some ring-shaped potentials (see, e.g. [19] and references therein).

The integral transform methods have proven to be useful and powerful for solving ordinary differential equations because they can convert the original equation into a simpler differential equation or into an algebraic equation. The Laplace transform method applied to quantum mechanics was used by Schrödinger into the discussion of radial eigenfunction of the hydrogen atom [58], and later Englefield approached the three-dimensional Schrödinger equation with diverse spherically symmetric potentials [59]. More than twenty years later the hydrogen atom was reexamined with the Laplace transform method [60]. Recently, some interest has been revived in searching bound-state solutions of the Schrödinger equation via Laplace transform method. For some years now one-dimensional problems with the  $1/x$  [61], Morse [62], generalized Morse [63], Dirac delta [64] and harmonic oscillator [65] potentials, three-dimensional problems with the singular harmonic oscillator, the singular Coulomb [66], some ring-shaped [67] potentials, and the  $D$ -dimensional harmonic oscillator [68], have been solved for the Laplace transform. With fulcrum on the relation mapping the behaviour of the eigenfunction near infinity and the Laplace transform near isolated singular points, Englefield [59] found the spectrum of three-dimensional problems by imposing that the radial eigenfunction vanishes at the origin. Englefield's recipe, spiced up with the relation mapping the behaviour of the eigenfunction near the origin and its corresponding transform near infinity, was used in Ref. [65] in order to obtain the complete set of bound-state solutions for the one-dimensional harmonic oscillator without using the closed-form solution for the Laplace transform. Furthermore, the class of problems was enlarged to include eigenfunctions satisfying homogeneous Neumann conditions at the origin.

In the present paper, the spiced Englefield's recipe is followed with attention restricted to systems that after factorizing the behaviour at the neighbourhood of special points, the second-order differential equation for the eigenfunction can be reduced to the confluent hypergeometric equation. Then is shown that all well-behaved eigenfunctions for that class of systems are expressed in terms of generalized Laguerre polynomials. Exactly solvable problems in this category include all the potentials mentioned in the first paragraph and the exactly soluble generalized Morse potential is used as an illustration.

## II. LAPLACE TRANSFORM AND A FEW OF ITS PROPERTIES

Let us begin with a brief description of the Laplace transform and a few of its properties [69]. The Laplace transform of a function  $\Phi$  is defined by

$$F(s) = \mathcal{L}\{\Phi\} = \int_0^\infty d\xi e^{-s\xi} \Phi(\xi). \quad (1)$$

If there is some positive constant  $\sigma$  such that  $\Phi$  does not increase faster than  $e^{\sigma\xi}$  for sufficiently large  $\xi$  then  $\Phi$  is said to be of exponential order  $\sigma$ . In this case, the integral in Equation (1) may exist for  $\text{Re } s > \sigma$ . Nevertheless, the Laplace transform may fail to exist because of a sufficiently strong singularity in the function  $\Phi$  as  $\xi \rightarrow 0$ . In particular,  $\xi^\lambda$  is of exponential order arbitrary and

$$\mathcal{L}\left\{\frac{\xi^\lambda}{\Gamma(\lambda+1)}\right\} = \frac{1}{s^{\lambda+1}}, \quad \text{Re } \lambda > -1, \quad \text{Re } s > 0, \quad (2)$$

where  $\Gamma$  is the gamma function. Derivative properties involving the Laplace transform are convenient for solving differential equations. In this paper we shall use the following properties:

$$\begin{aligned} \mathcal{L}\left\{\frac{d\Phi}{d\xi}\right\} &= sF(s) - \Phi|_{\xi=0} \\ \mathcal{L}\left\{\frac{d^2\Phi}{d\xi^2}\right\} &= s^2F(s) - s\Phi|_{\xi=0} - \frac{d\Phi}{d\xi}\Big|_{\xi=0} \\ \mathcal{L}\{\xi\Phi\} &= -\frac{dF(s)}{ds}. \end{aligned} \quad (3)$$

More than this, we shall use a pair of relations mapping limiting forms. If near an isolated singular point  $s_0$  the Laplace transform behaves as

$$F(s) \underset{s \rightarrow s_0}{\sim} \frac{1}{(s - s_0)^\nu}, \quad \nu > 0, \quad (4)$$

then

$$\Phi(\xi) \underset{\xi \rightarrow \infty}{\sim} \frac{1}{\Gamma(\nu)} \xi^{\nu-1} e^{s_0 \xi}. \quad (5)$$

On the other hand,

$$\lim_{s \rightarrow \infty} sF(s) = \Phi(0), \quad (6)$$

an result known as initial value theorem.

### III. THE GENERALIZED MORSE POTENTIAL

The time-independent Schrödinger equation is an eigenvalue equation for the characteristic pair  $(E, \psi)$  with  $E \in \mathbb{R}$ . For a particle of mass  $m$  embedded in the generalized Morse potential it reads

$$\frac{d^2 \psi(x)}{dx^2} + \frac{2m}{\hbar^2} (E - V_1 e^{-\alpha x} - V_2 e^{-2\alpha x}) \psi(x) = 0, \quad (7)$$

where  $\hbar$  is Planck's constant,  $\alpha > 0$ , and  $\int_{-\infty}^{+\infty} dx |\psi|^2 = 1$  for bound states. The substitution

$$\xi = \frac{2\sqrt{2mV_2} e^{-\alpha x}}{\hbar\alpha} \quad (8)$$

and the definitions

$$S = \frac{\sqrt{-2mE}}{\hbar\alpha}, \quad a = \frac{mV_1}{\hbar\alpha\sqrt{2mV_2}} + S + \frac{1}{2} \quad (9)$$

convert Eq. (7) into

$$\frac{d^2 \psi(\xi)}{d\xi^2} + \frac{1}{\xi} \frac{d\psi(\xi)}{d\xi} + \left( -\frac{1}{4} + \frac{S - a + 1/2}{\xi} - \frac{S^2}{\xi^2} \right) \psi(\xi) = 0, \quad (10)$$

whose solutions have asymptotic limits expressed as  $\psi(\xi) \xrightarrow{|\xi| \rightarrow 0} \xi^{\pm S}$  and  $\psi(\xi) \xrightarrow{|\xi| \rightarrow \infty} e^{\pm \xi/2}$ .

On account of the normalization condition,  $\int_0^\infty d|\xi| |\psi(\xi)|^2 / |\xi| = \alpha$ , one has that  $\psi$  behaves like  $\xi^S$  as  $|\xi| \rightarrow 0$  and like  $e^{-\xi/2}$  as  $|\xi| \rightarrow \infty$  with  $\xi \in \mathbb{R}$  ( $V_2 > 0$ ) and  $S > 0$  ( $E < 0$ ). The substitution

$$\psi(\xi) = e^{-\xi/2} \xi^S \Phi(\xi) \quad (11)$$

transforms Eq. (10) into

$$\xi \frac{d^2 \Phi(\xi)}{d\xi^2} + (b - \xi) \frac{d\Phi(\xi)}{d\xi} - a \Phi(\xi) = 0, \quad (12)$$

with  $b = 2S + 1 > 1$ . Eq. (12) is the standard form of the confluent hypergeometric equation [70]. Notice that  $\Phi$  is a nonzero constant at the origin and tends to infinity no more rapidly than  $\exp(\sigma_1 \xi^{\sigma_2})$ , with  $\sigma_2 < 1$  and arbitrary  $\sigma_1$ , for sufficiently large  $\xi$ . This occurs because  $\sigma_1 \xi^{\sigma_2} - \xi/2 \rightarrow -\xi/2$  as  $\xi \rightarrow \infty$ . The regular behaviour of  $\Phi$  at the origin plus its behaviour for large  $\xi$  ensure the existence of its Laplace transform. In this case  $\Phi$  is of exponential order arbitrary and consequently its Laplace transform exists for  $\text{Re } s > 0$ .

#### IV. LAPLACE TRANSFORM OF THE CONFLUENT HYPERGEOMETRIC EQUATION

Using the derivative properties of the Laplace transforms given by (3), the confluent hypergeometric equation is mapped onto

$$s(s-1) \frac{dF(s)}{ds} + [(2-b)s + a - 1] F(s) = (1-b) \Phi(0), \quad \text{Re } s > 0. \quad (13)$$

Note that this first-order differential equation has regular (nonessential) singularities at  $s = 0$  and  $s = 1$ . Therefore,  $F(s)$  is either analytical, or possess a pole or branch point, at the regular singular point (Fuchs theorem). The relation connecting the behaviour of  $F$  near an isolated singular point and the behaviour of  $\Phi$  for large  $\xi$  dictates that  $\Phi$  behaves like  $\xi^{\nu-1}$  or  $\xi^{\nu-1} e^\xi$ , depending on where the isolated singularity of  $F$  is, whether near  $s = 0$  or  $s = 1$ , respectively. Due to the asymptotic behaviour prescribed for  $\Phi$  at the end of the previous section, one sees that  $F$  behaves like  $s^{-\nu}$  as  $s \rightarrow 0$ , and (13) enforces

$$\nu = 1 - a. \quad (14)$$

On the other hand, using the initial value theorem one sees that  $F$  behaves like  $\Phi(0)/s$  as  $s \rightarrow \infty$ . Thus, we seek a particular solution of (13), regular at  $s = 1$ , in the form of a polynomial in inverse powers of  $s$ :

$$F(s) = \sum_{j=0}^n c_j s^{j-\nu} = \frac{c_0}{s^\nu} + \cdots + \frac{c_n}{s}, \quad (15)$$

with  $c_0 \neq 0$  and

$$\nu = n + 1, \quad (16)$$

in such a way that  $s = 0$  is a pole of order  $n + 1$  and  $F(s)$  is the principal part of a finite Laurent series with residue  $c_n = \Phi(0)$  at  $s = 0$ . Comparing (14) with (16), one sees that

$$a = -n. \quad (17)$$

Substituting (15) into (13) one obtains the following two-term recursive relation for the coefficients

$$c_{j+1} = c_j \frac{1 + j - n - b}{j + 1}, \quad j \geq 0. \quad (18)$$

Inspection and induction yields

$$c_j = c_0 \frac{(-1)^j}{j!} \frac{\Gamma(n + b)}{\Gamma(n + b - j)}, \quad 0 \leq j \leq n. \quad (19)$$

This means that

$$F(s) = c_0 \sum_{j=0}^n \frac{(-1)^j}{j!} \frac{\Gamma(n + b)}{\Gamma(n + b - j)} s^{j-n-1}. \quad (20)$$

Using (2), the termwise inverse transformation of (20) leads to the polynomial solution for  $\Phi$ :

$$\Phi(\xi) = c_0 \sum_{j=0}^n \frac{(-1)^j}{j!} \frac{\Gamma(n + b)}{\Gamma(n + b - j)(n - j)!} \xi^{n-j}. \quad (21)$$

Then, using Leibniz's formula for the generalized Laguerre polynomials [70]

$$L_n^{(b-1)}(\xi) = \sum_{j=0}^n \frac{\Gamma(n + b)}{\Gamma(j + b)} \frac{(-\xi)^j}{j!(n - j)!}, \quad b > 0, \quad (22)$$

one obtains

$$\Phi_n(\xi) = c_0 (-1)^n L_n^{(b-1)}(\xi). \quad (23)$$

Actually, condition (17) transforms the confluent hypergeometric equation into generalized Laguerre's equation in such a way that the succeeding process involving the inversion of the Laplace transform is not surprising.

For systems whose eigenfunctions can be expressed in terms of a particular solution of the confluent hypergeometric equation, Eqs. (17) and (23) summarize all we need to determine the complete set of bound-state solutions.

## V. BOUND STATES IN A GENERALIZED MORSE POTENTIAL

We now turn our attention to the generalized Morse potential. Substitution of (17) into (9) leads to the quantization condition

$$n + S + \frac{1}{2} = -\frac{mV_1}{\hbar\alpha\sqrt{2mV_2}}. \quad (24)$$

Hence,  $V_1 < 0$  so that the generalized Morse potential is able to hold bound states only if it has a well structure ( $V_1 < 0$  and  $V_2 > 0$ ). Furthermore, because  $E < 0$  one gets

$$n < \frac{m|V_1|}{\hbar\alpha\sqrt{2mV_2}} - \frac{1}{2}. \quad (25)$$

This restriction on  $n$  limits the number of allowed states and requires  $m|V_1|/(\hbar\alpha\sqrt{2mV_2}) > 1/2$  to make the existence of a bound state possible. Finally, we use the quantization condition (24) to write

$$E_n = -\frac{V_1^2}{4V_2} \left[ 1 - \frac{\hbar\alpha\sqrt{2mV_2}}{m|V_1|} \left( n + \frac{1}{2} \right) \right]^2. \quad (26)$$

With the generalized Laguerre polynomial standardized as [70]

$$L_n^{(\mu)}(z) = \sum_{j=0}^n \frac{\Gamma(n+\mu+1)}{\Gamma(j+\mu+1)} \frac{(-z)^j}{j!(n-j)!} \quad (27)$$

and the integral [71]

$$\int_0^\infty dz e^{-z} z^{\gamma-1} L_n^{(\mu)}(z) = \frac{\Gamma(\gamma)\Gamma(1+\mu+n-\gamma)}{n!\Gamma(1+\mu-\gamma)}, \quad \text{Re } \gamma > 0, \quad (28)$$

one can show that

$$\int_0^\infty dz e^{-z} z^{\mu-1} [L_n^{(\mu)}(z)]^2 = \frac{\Gamma(\mu+n+1)}{\mu n!}, \quad \text{Re } \mu > 0. \quad (29)$$

Therefore, the normalization condition yields the normalized eigenfunction (firstly obtained in Ref. [7] for  $V_2 = -2V_1$ ):

$$\psi_n(\xi) = \sqrt{\frac{2\alpha S n!}{\Gamma(2S+n+1)}} \xi^S e^{-\xi/2} L_n^{(2S)}(\xi). \quad (30)$$

## VI. CONCLUDING REMARKS

Bessel's equation as well as differential equations with linear coefficients can be mapped onto simpler homogeneous first-order differential equations for the Laplace transform when the original functions are subject to special boundary conditions at the origin (see, e.g. [69]). Following the spiced Englefield's recipe, we have shown that the bound-state solutions of the Schrödinger equation whose eigenfunctions are expressed in terms of particular solutions of the confluent hypergeometric equation, including the large class of systems with potentials relevant to atomic and molecular physics such as the generalized Morse, singular harmonic oscillator, and singular Coulomb potentials, beyond the ring-shaped potentials approached in Ref. [67], can be obtained by using the Laplace transform of the confluent hypergeometric equation. In those cases, the Laplace transform maps the confluent hypergeometric equation onto a nonhomogeneous first-order differential equation. The source of nonhomogeneity is just the particular solution of the confluent hypergeometric equation at the origin but this fact does not represent a less favourable position because it is related asymptotically to the residue of the Laplace transform at the origin via the initial value theorem. It is worthwhile recall that the eigenfunction for the generalized Morse potential does not have values prescribed at the origin. The spiced Englefield's recipe allows searching for a particular solution of the transformed equation with a well-defined singularity and a well-defined asymptotic behaviour, and such as presented in this paper the exact-closed form of the Laplace transform does not have relevance to determinate the complete set of bound-state solutions.

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